TITLE: **Mathematically Reduced Chemical Reaction Mechanism Using Neural Networks**

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1.ABSTRACT

Program Introduction: Rationale and Objectives

The aim of the project is to develop an efficient chemistry model for combustion simulations. The reduced chemistry model will be developed mathematically without the need of having extensive knowledge of the chemistry involved. To aid in the development of the model, Neural Networks (NN) will be used via a new network topology know as Non-linear Principal Components Analysis (NPCA). This is a continuation of work started in a previously DOE funded Faculty/Student exploratory research.

Many Combustion systems are modeled by very high-dimensional systems of non-linear differential equations. These equations often exhibit solutions which are un-evenly distributed in phase-space, and which may exist as circles, tori or other manifolds. It is desirable to approximate these isolated regions of the phase-space by a mathematical model of lower dimension than the dimension of the original ambient space. NPCA accomplishes this task using NN.

Accomplishments Achieved During the Current Period of Performance:

In a previous investigation, it was found that the NPCA developed was hard to train as well as slow in converging to the optimal solution. For this reason, the initial objectives of the project, is to develop ways and means of accelerating training and convergence of NPCA. The difficult in training is due to the fact that NN training is an ill-posed non-linear optimization problem and as such has problems with local minima, slow convergence as well as stability with respect to errors in input data. To address these problems, we have looked at several techniques intended to improve training of NPCA. During this period we have looked at: (i) data transformation techniques applied to input data, (ii) a spectrum based training method which allows a network to train faster. Here, the spectrum of the output layer is compared to the spectrum of the output of the hidden layers with the information used to minimize the error between the function solution and the network and (iii) Generalized Regression Neural Network,(GRNN). This method is based on Bayes probabilistic theory and maybe quite promising. Here only one pass of the training data set is required. It is said to be excellent with sparse data sets and have outperformed backpropagation in previous tests.

Another objective addressed during this period is how to generate efficient training data for the NPCA. We have studied the statistical technique of Bagging (Bootstrap AGGregatING) and believe that this will be the best method to use with NPCA. In this method, if there are n, variables of the data, then n, training samples are generated at random and used to train a NPCA. Each training sample is used to develop a different NPCA model. The overall reduced model of the reaction mechanism, will be a combination of the reduced models of all NPCA models developed. This method will be compared to the standard Design of Experiments technique.

Plans for the Remaining Period of Performance

The remaining tasks in this project include**:**

- Develop an efficient training method for NPCA
- Implement Bagging method to generate training data
- Develop the NPCA model on real chemical reaction mechanism data
- Couple NPCA model to a CFD code. Code chosen is the popular KIVA combustion simulation code**.**

2. LIST OF PUBLICATIONS AND STUDENTS SUPPORTED

Publications

- Non during this period

Students Supported

- Ken Johnson, who is a beginning graduate student in applied mathematics
- Owen Clark, an undergraduate senior.